Material and Energy Balance Computations
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Lecture –29
Single Phase Systems (Contd.,)

Hello everyone, Welcome back in the NPTEL online certification course on material and energy balance computations. We were discussing the single phase system the concept of partial pressure.

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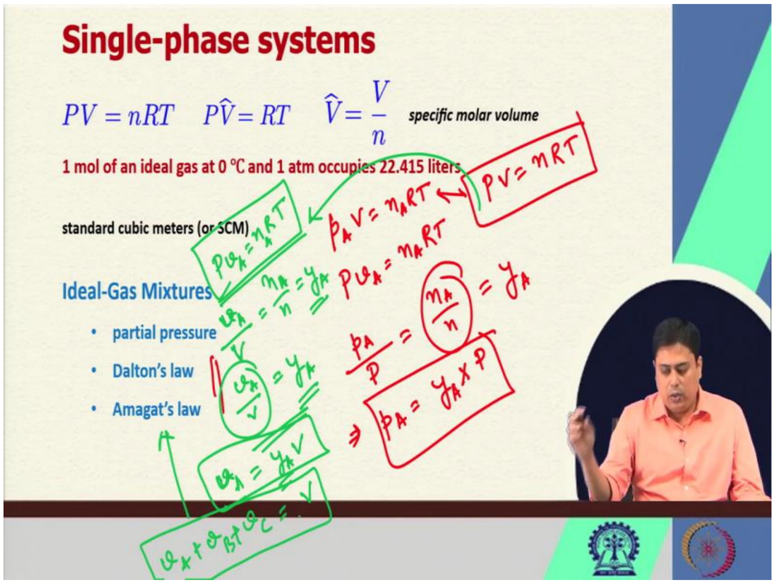

Single-phase systems

$PV = nRT$ $P\hat{V} = RT$ $\hat{V} = \frac{V}{n}$ specific molar volume

1 mol of an ideal gas at 0 °C and 1 atm occupies 22.415 liters

standard cubic meters (or SCM)

Ideal-Gas Mixtures

- partial pressure
- Dalton's law
- Amagat's law

$PV = nRT$

$p_A V = n_A RT$

$P v_A = n_A RT$

$\frac{p_A}{P} = \frac{n_A}{n} = y_A$

$p_A = y_A \times P$

$P v_A = n_A RT$

$\frac{v_A}{V} = \frac{n_A}{n} = y_A$

$\frac{v_A}{V} = y_A$

$v_A = y_A V$

$v_A + v_B + v_C = V$

And we have realized that the partial pressure of a substance of a pure substance is basically its mole fraction times the total pressure of the system. Now this y_A that is here we know that. Now similarly for component B we can write y_B times P, $P_C = y_C \times P$ etc, or similarly like this. At the same time we are now aware that the mole fractions the summation of it should be one. So, if we add all these what we have is basically the partial pressures of components in an ideal gas on the left hand side is equals to these terms.

The summation of, what we got here $P_B + P_C = y_A + y_B + y_C \times P_{tot}$. Now this is one. So, what we have that means the summation of the total the partial pressures of the individual components in an ideal gas mixture yields to the total pressure of the system and that is the Dalton's law. Now the similar thing we can derive for when we have instead of change in pressure we have the volume that the volume it would occupy a pure substances occupy if the system remains at temperature T and pressure P in a moles of that pure component.

The amount of volume or the size of the volume that would it occupies if it were left alone in the mixture or there is no mixture as such. So, now in this case if we divide this by this PV = nRT what we have is basically v_A by capital V = n_A / n which is again this is a mole fraction. Now here you now realize that this is the volume fraction the amount of component A in the mixture divided by the total volume is the volume fraction of that component which is equals to its mole fraction.

Now this is very important thing and that is why if any problem statement says that the gas mixtures are by this percentages or the gas mixture components composition is known to you in volume % and that gas mixture behaves ideally or as a ideal gas. Then those fractions or those percentages can directly be interpreted as the mole fraction of the mole percentages which helps in our calculation.

So, that is why the gaseous components whenever we deal with if the problem statement in anywhere it is mentioned as the volume fraction and if it behaves as ideal gas we consider those values directly as the mole fraction because of this reason. Now here the thing is that similar to our previous concept we have $v_A = y_A V$. So, similarly $v_A + v_B + v_C = V$ because summation of y_i for i = 1 to n, it is one.

So this volume additive nature that the volume fraction of each and every component eventually consist the whole volume of the system is called the Amagat's law when we have the pressures the partial pressures adds up to the total pressure of the system is the Daltons law. The volume fraction adds up to give the total volume is the Amagat's law.

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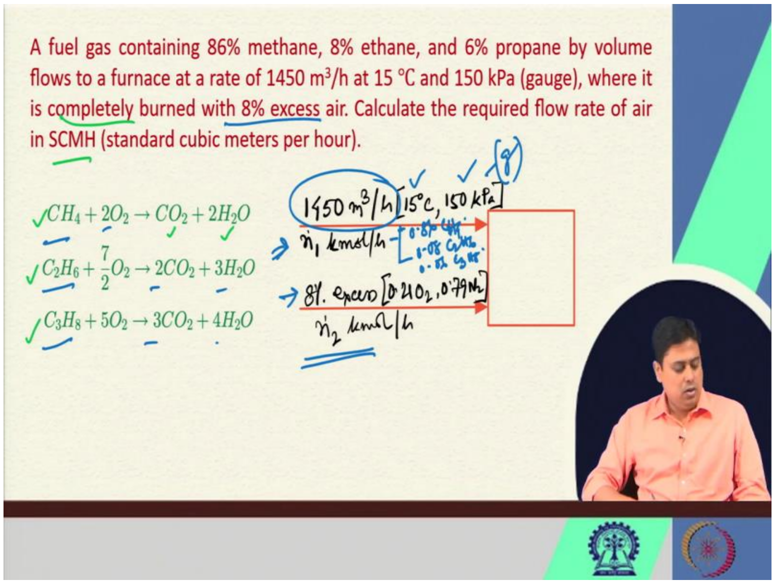

A fuel gas containing 86% methane, 8% ethane, and 6% propane by volume flows to a furnace at a rate of 1450 m^3/h at 15 °C and 150 kPa (gauge), where it is completely burned with 8% excess air. Calculate the required flow rate of air in SCMH (standard cubic meters per hour).

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

$C_2H_6 + \frac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O$

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

Now say look at this example and we see that whatever we have now discussed how we apply that in solving the problems. So, this is again a combustion problem but now here this term is introduced. The problem statement says that we have a fuel gas that contains 86% methane, 8% ethane and 6% propane by volume and flows to a furnace at a rate of 1450 m^3/h at 15 °C and 150 kPa gauge pressure where it is completely burnt with 8% excess air.

We have to calculate the required flow rate of air in standard cubic meters per hour that is SCMH. So how do we solve such problem the first thing is that now here we understand the problem once again that there is a fuel gas its composition are known the compositions are of hydrogen and carbon that is the hydrocarbon fuel. It is completely burned in presence of excess air the flow rate is known but the flow rate is given at a different temperature than the standard temperature and pressure.

So, we have to find out what is the required flow rate of air at standard temperature and pressure. So, for that we at first write the complete combustion reactions because it is written that it is completely burned that is complete combustion is happening in presence of excess air and in case of complete combustion. Now we know there will be only CO_2 and water, complete combustion of carbon produces CO_2 complete conversion of hydrogen creates H_2O and then we write the stoichiometric coefficients appropriately in a balanced manner because this stoichiometry will give us the necessary information.

So, methane, ethane and propane. so, we have the reactions this tells that one mole of methane requires 2 moles of oxygen for complete combustion. One mole of ethane requires 3.5 moles of oxygen one mole of propane requires 5 moles of oxygen and by this stoichiometric coefficient it generates that amount of carbon dioxide and water. We draw the flow chart, so that we can write all the necessary information here on the flowchart and we need not look back again and again to the problem statement.

So, here what we have that there is a fuel gas that is flowing at this rate at this temperature and pressure do not forget to write this information and then only you can understand whether the conversion is necessary or not because if the product stream is required at a different temperature and pressure that can easily be identified if you had written this information here. So, it is 15 degree centigrade and 150 kPa that is gauge pressure.

It is incomplete till now because I have not mentioned this 86%, 8% and 6% composition. So, here you must write the compositions like 0.86 CH_4, 0.08 C_2H_6 and 0.06 C_3H_8, this much mole of CH_4 per mole of this gas component gas mixture. The second stream that we have we have 8% excess air and we do not know what is the number of moles or the molar flow rate of that stream.

So, we write that this is also we write here instead of immediately calculating this. This air consists of oxygen and nitrogen since it is explicitly not mentioned what is the composition of air. So, it is 0.21 that means one mole of this air consist 0.21 moles of oxygen and 0.79 moles of nitrogen. So, that is written here in compact form, which is 21% oxygen and 79% nitrogen in this excess air.

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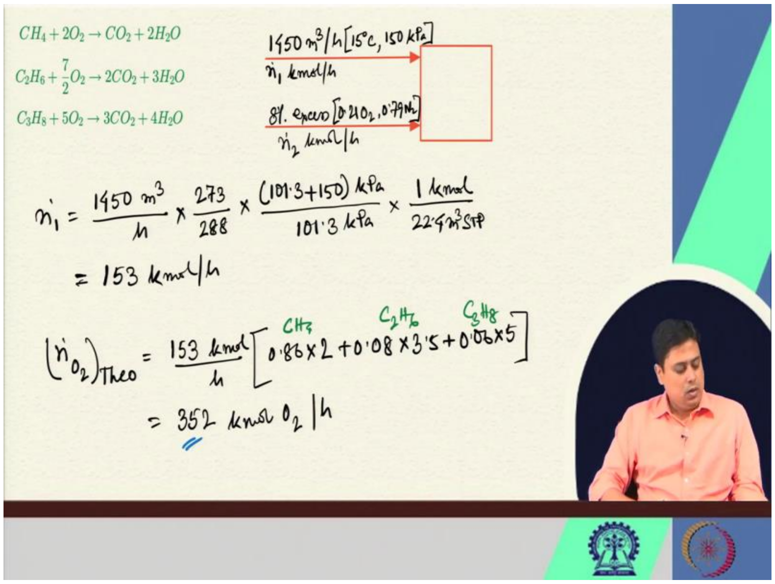

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$$\dot{n}_1 = \frac{1450\ m^3}{h} \times \frac{273}{288} \times \frac{(101.3+150)\ kPa}{101.3\ kPa} \times \frac{1\ kmol}{22.4\ m^3\ STP}$$

$$= 153\ kmol/h$$

$$(\dot{n}_{O_2})_{Theo} = \frac{153\ kmol}{h}\left[\overset{CH_4}{0.86\times 2} + \overset{C_2H_6}{0.08\times 3.5} + \overset{C_3H_8}{0.06\times 5}\right]$$

$$= 352\ kmol\ O_2/h$$

So that means now if we proceed to the problem you must be doing the degree of freedom analysis quickly let us go to the problem solution. So, here this is the set of reaction this is the flow diagram. The first thing that we can do is the conversion of this because we assume now here that this thing behaves as ideal gas, this mixture. So, the moles or the molar flow rate or that we calculate here is basically 1450 m^3/h this is the actual flow rate at this temperature and pressure remember PV = nRT relation T is the absolute temperature.

So, the zero degree means 0°C means it is 273 K, 273 + 15 it is 288 K. So, we basically convert this value from this temperature and pressure to the standard temperature and pressure which is 0 degree centigrade which means 273 Kelvin and 1 atm which is 101.3 kPa. Remember 150 was the gauge pressure it has to be converted to absolute pressure.

So, gauge pressure plus atmospheric pressure is our absolute pressure which is done here. So, this part is basically the conversion of this volume from this temperature pressure to zero degree centigrade and this pressure, once we convert this we know that one kmol of ideal gas would occupy 22.4 m^3 of volume or in other words I have shown you earlier that one mole of ideal gas occupies 22.4 litre of the volume.

So, if you just make an unit conversion from mole to kilo mole it becomes 22.4 liter to 22.4 m^3 at STP. So, this volume we converted the volume from this temperature to this temperature then this volume we converted to the number of moles. Because this volume would occupy how much mole that is our answer for this part or the calculation of n_1 which is approximately or numerically close to 153 kmol/h.

So, then we look for the amount of oxygen that is theoretically required. Because now we know the amount of fuel is completely burning for which we need to know how much oxygen is required. Now theoretical requirement is for the complete combustion always. So, once we have this much amount of fuel per hour flowing and in this fuel you have 86% of methane and in that methane or that methane requires 2 moles of oxygen for complete combustion.

So, it is ×2, so, 153 × 0.86 is the number of mole of methane is completely burning. Now that amount of methane requires × 2 this mole of oxygen this is the expression. Similarly you have ethane which is 0.08 × 153 this much of ethane it requires ×3.5 moles of oxygen because one mole of ethane requires 3.5 moles of oxygen.

And so, for the propane 153 × 0.06 because this is the compositions that we have that is 6% of propane is there in the mixture and 1 mole of propane requires 5 moles of oxygen. So, it is × 5. This is my total theoretical requirement of oxygen for complete combustion, which if we numerically calculate it is numerically close to 352 kmol of oxygen per hour.

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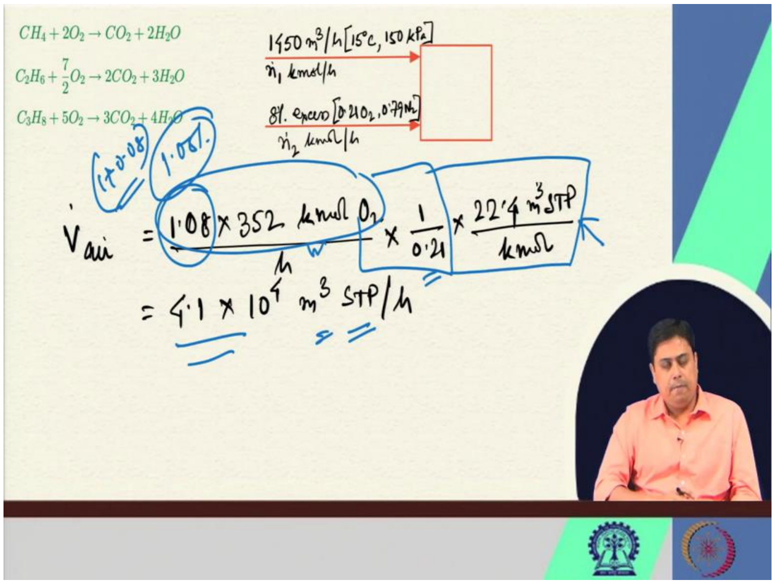

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$$\dot{V}_{air} = \frac{\boxed{1.08} \times 352\ \text{kmol } O_2}{h} \times \frac{1}{0.21} \times \frac{22.4\ m^3\ STP}{kmol}$$

$$= 4.1 \times 10^4\ m^3\ STP/h$$

Once we have it we need to know, what is the amount of air being flown to the system or being fed to the system. We know for the oxygen, and we know that air consists of 21 mole percent oxygen. So, the amount of oxygen theoretically needed multiplied by 8% excess this is one plus 0.08 because 8% excess air is fed to the system that is mentioned. So, this means this is the excess amount of oxygen being fed to the system per hour. Now one mole of air consists 0.21 moles of oxygen.

So, this much oxygen would be there in this amount of air once this moles of air is known we multiply that with 22.4 meter cube because this mole would be there if the volume is of this much because we know that 22.4 meter cube volume is occupied by 1kmol of the gas mixture because it is behaving as if a ideal gas. So, from oxygen calculation we basically converted to the air requirement the moles of air that moles of air would be in how much volume that we did with this conversion.

And that is why earlier I mentioned that you need to remember this 22.4 number because it is essential that you remember that one mole of ideal gas would occupy 22.4 liter of the volume or 1kmol of ideal gas at zero degree centigrade and one atmosphere would occupy 22.4 meter cube of volume. So, this helps us quickly converting the volume and number of moles and eventually we get this numerical value that it is 4.1×10^4 m^3/h at standard temperature and pressure here the standard temperature and pressure zero degree centigrade and 1 atmosphere pressure.

So, I hope this problem is or the solution of this problem is very clear to you how we are using this information that we have learnt and here directly we have interpreted this number which is by volume to the mole fractions of the molar conversion the molar numbers the number of moles or the mole composition.

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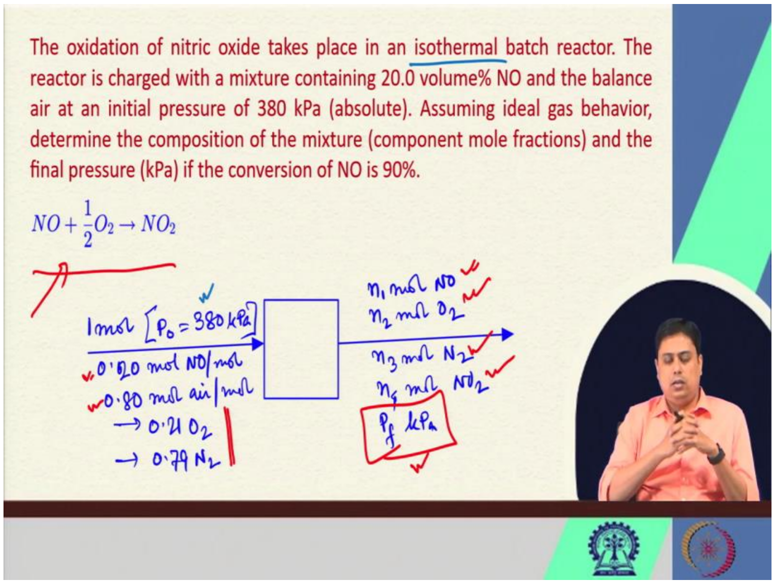

The oxidation of nitric oxide takes place in an isothermal batch reactor. The reactor is charged with a mixture containing 20.0 volume% NO and the balance air at an initial pressure of 380 kPa (absolute). Assuming ideal gas behavior, determine the composition of the mixture (component mole fractions) and the final pressure (kPa) if the conversion of NO is 90%.

$NO + \frac{1}{2}O_2 \rightarrow NO_2$

So, if we now move on to the next problem which says that the oxidation of nitric oxide takes place in an isothermal batch reactor here isothermal batch reactor means the temperature is not changing the reactor is charged with a mixture containing 20 volume percent nitric oxide and the balance air at an initial pressure of 380 kPa absolute, assuming ideal gas behavior determine the temperature of the composition of the mixture that is the component mole fractions and the final pressure in kPa if the conversion of nitric oxide is 90%.

So, how do we do such problem? So, the first step again we write the reaction with balanced stoichiometry that is the nitric oxide plus half O_2 giving us NO_2, we have to draw the flowchart or the flow diagram for it. Now here what is happening the reactor is charged with a mixture of certain amount of nitric oxide and air which means in the feed we have oxygen nitrogen and NO there is a certain conversion of NO which means the NO is not completely reactive.

So, we have some excess of NO that would come out from the system. So, in the product stream what we will have, will have NO, we have oxygen, we have nitrogen and we will have NO_2 there would be no question of moisture or water because there is no hydrogen component is there in the inlet or the input stream but the question is what is the final pressure if the conversion is 90%. So, our flow chart or the flow diagram would look like something like this provided we consider the basis of calculation as one mole of the feed.

So, if the feed is of one mole it is a batch reactor that that is why there is no flow rate mentioned. So, one mole of feed is particularly fed into this particular reactor at an initial pressure of 380 kPa there the composition is 0.2 mole of NO and the rest is air and in air we have 21% oxygen and 79% nitrogen the output stream as we have analyzed the unknowns are number of moles of NO, number of moles of O_2, number of moles of N_2, number of moles of N_2O, this is at P final unknown pressure. We have to find out what is this value.

So before I solve this problem I want you to do this yourself and in the next class I will show its solution. This is again a pretty simple problem if you have understood the concepts that we have discussed till now this should not be a problem in solving it. Remember here the reaction is of only one reaction that is happening. So, if you now remember that which method I would apply because in the last problem we have just balanced the number of moles and here basically we have converted the moles the volumes we have interchangeably did that.

We have not used any balance in those system basically in the say the 3 of the methodologies that we have learnt that is either molecular species balance, atomic species balance, or chemical reaction extent, extent of reaction mechanism. There was no reactions were involved but here now we have one reaction and even if there was reactions involved the point although here reactions are involved.

But the question was framed in such a way that we did not have to do any material balance. We just learnt the conversion of volume and moles. But here we have to now apply the combination of reactive species balance along with the ideal gas law. So, we will see the solution in the next class but mean while I would like you to do this problem or the solution of this problem by yourself. Thank you for your attention and will see you in the next class.